

ARMY RESEARCH LABORATORY



# Derivation of Effective-Mass Expressions for Electrons and Holes in the Anisotropic Multiband Semimetals Ar, Sb, and Bi

Frank J. Crowne

ARL-TR-2152

August 2000

Approved for public release; distribution unlimited.

DIGITAL QUALITY INSPECTED 4

20000829 169

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorized documents.

Citation of manufacturer's or trade names does not constitute an official endorsement or approval of the use thereof.

Destroy this report when it is no longer needed. Do not return it to the originator.

# **Army Research Laboratory**

Adelphi, MD 20783-1197

---

ARL-TR-2152

August 2000

---

## **Derivation of Effective-Mass Expressions for Electrons and Holes in the Anisotropic Multiband Semimetals Ar, Sb, and Bi**

Frank J. Crowne

Sensors and Electron Devices Directorate

---

## **Abstract**

---

In this report, certain properties of the multicomponent plasmas present in the group-V semimetals As, Sb, and Bi have been derived. Notable among these properties is anisotropy of the effective masses of both electrons and holes, which in turn leads to anisotropy in the plasma frequencies of these materials. Because the systems of interest are particles in a host matrix rather than bulk materials, it is likely that this anisotropy in the plasma response will be averaged out in some way; however, this problem must be examined in detail before such a conclusion is warranted.

---

## Contents

---

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>Boltzmann-Equation Calculation of Fermi Velocities in Group-V Semimetals</b>	<b>2</b>
<b>3</b>	<b>Calculations of Sums Over <math>k</math>-Space Minima for High-Symmetry Band Structures</b>	<b>10</b>
3.1	Simple Cubic Band Structure . . . . .	10
3.2	(111) Cubic Pockets (Tetrahedral Band Structure) . . . . .	11
<b>4</b>	<b>Calculations of Sums Over <math>k</math>-space Minima for the Band Structures of Group-V Elements</b>	<b>14</b>
<b>5</b>	<b>Conclusions</b>	<b>17</b>
	<b>References</b>	<b>18</b>
	<b>Distribution</b>	<b>19</b>
	<b>Report Documentation Page</b>	<b>21</b>

## Figures

1	Conduction band minima (pockets) of silicon in $k$ -space. . . . .	10
2	Conduction band minima (pockets) of germanium in $k$ -space. .	11
3	Conduction-band and valence-band minima (pockets) of As and Sb in $k$ -space . . . . .	14

---

## 1. Introduction

---

The electrodynamic properties of the semimetallic group-V elements (arsenic, antimony, and bismuth) are complex and ill-understood in many ways. This is primarily due to the complicated structures of their conduction and valence bands, which have many maxima and minima for the Fermi surface to intersect, resulting in multiple “pockets” of electrons and holes populated by carriers at all temperatures [1]. According to the Sommerfeld theory of metals, each minimum or maximum should give rise to a different species of electron or hole, so that the electrodynamic response of the material resembles that of a multicomponent plasma. To make matters worse, all these materials crystallize orthorhombically, so that their charge carriers (both electrons and holes) have anisotropic effective masses.

When nanometer-size samples of these materials (so-called *quantum dots*) are prepared, the resulting systems are expected to behave in unusual ways when probed by electromagnetic radiation. A particularly easy way to create such samples was discovered some 10 years ago, when researchers found that under certain conditions low-temperature growth of GaAs by molecular-beam epitaxy (MBE) resulted in material with large numbers of ultramicroscopic inclusions of As, up to 1 percent of the host volume [2], which arose from the aggregation of  $\text{Ga}_{\text{As}}$  antisite defects (i.e., lattice sites at which a gallium atom was replaced by an As atom). Although theories regarding their nature are still problematic, there are strong indications that these inclusions, which are roughly spherical in shape, consist of metallic arsenic. Similar behavior has been observed when InAs and GaSb are grown in this way.

There is ample reason to believe that these materials could be useful in device engineering. However, before this usefulness can be explored, the individual nanoparticles must be properly modeled with regard to interactions with electromagnetic waves. In this report, I derive an appropriate set of constitutive equations that can be used with the Maxwell equations to implement this modeling.

---

## 2. Boltzmann-Equation Calculation of Fermi Velocities in Group-V Semimetals

---

The most effective way to deal with metals and their interactions with electromagnetic radiation (light, microwaves, etc) is to use the Boltzmann-Vlasov equation to calculate momentum ( $k$ -space) distributions for the metallic charge carriers [3]. For semimetals, this naturally leads to a general multiband set of Boltzmann equations:

$$\partial_t f_j + v_\alpha^{(j)}(\vec{k}) \partial_\alpha f_j + \frac{e}{\hbar} (\partial_\alpha \phi) \left( \frac{\partial}{\partial k_\alpha} f_j \right) = -\frac{1}{\tau_j} \left( f_j - \frac{n_0^{(j)}}{n_0^{(j)}} f_0^{(j)}(\vec{k}) \right), \quad (1)$$

where  $f^{(j)}(\vec{k}, \vec{x}, t)$  is the number distribution function for the  $j$ th carrier,  $v_\alpha^{(j)}(\vec{k})$  is the semiclassical (hydrodynamic) velocity of such a carrier with momentum  $k$ ,  $\tau_j$  is its particle-number-conserving relaxation time, and  $\phi(x, t)$  is any external (electrostatic) potential applied to the system. The hydrodynamic approximation introduces a parameterization of the solutions to these equations in terms of macroscopic variables such as density, drift velocity, etc, which are determined self-consistently as moments of the equations. If the particles are semiconducting with parabolic bands, we can use Maxwell-Boltzmann functions for the perturbed carrier distributions:

$$f^{(j)}(\vec{k}, \vec{x}, t) = 4\pi^3 n^{(j)}(\vec{x}, t) \left[ m_l m_t^2 \right]^{-1/2} \left( \frac{\hbar^2}{2\pi k_B T^{(j)}(\vec{x}, t)} \right)^{3/2} \exp \left\{ -\frac{1}{kT^{(j)}(\vec{x}, t)} G^{(j)}(\vec{k}, \vec{x}, t) \right\}, \quad (2)$$

where

$$G^{(j)}(\vec{k}, \vec{x}, t) = \frac{\hbar^2}{2} \left( \vec{k} - \vec{k}_D^{(j)}(\vec{x}, t) - \vec{k}_{0j} \right)_\alpha \left[ m_j^{-1} \right]_{\alpha\beta} \left( \vec{k} - \vec{k}_D^{(j)}(\vec{x}, t) - \vec{k}_{0j} \right)_\beta. \quad (3)$$

Here  $n^{(j)}(\vec{x}, t)$  is the hydrodynamic density of carriers in the  $j$ th carrier pocket,  $\vec{k}_D^{(j)}(\vec{x}, t)$  is the hydrodynamic drift momentum of carriers in this pocket,  $k_{0j}$  locates the center of the pocket in  $k$ -space,  $m_j^{-1}$  is the effective-mass tensor of the  $j$ th carrier type with principal values  $m_l$  and  $m_t$  (assuming the pockets are spheroidal),  $k_B$  is Boltzmann's constant,  $T^{(j)}(\vec{x}, t)$  is the hydrodynamic temperature of the  $j$ th carrier type, and  $\hbar$  is Planck's constant. The corresponding unperturbed distributions are

$$f_0^{(j)}(\vec{k}) = 4\pi^3 n_0^{(j)} \left[ m_l m_t^2 \right]^{-1/2} \left( \frac{\hbar^2}{2\pi k_B T} \right)^{3/2} \exp \left\{ -\frac{\hbar^2}{2kT} \left( \vec{k} - \vec{k}_{0j} \right)_\alpha \left[ m_j^{-1} \right]_{\alpha\beta} \left( \vec{k} - \vec{k}_{0j} \right)_\beta \right\}, \quad (4)$$

where  $n_0^{(j)}$  is the equilibrium density of carriers in the  $j$ th carrier pocket, and  $T$  is the usual lattice temperature. For metallic particles, the correct distributions at low temperatures are perturbed Fermi distributions:

$$f^{(j)}(\vec{k}, \vec{x}, t) = \theta\left(\epsilon_F(\vec{x}, t) - \epsilon_{Pj} - G^{(j)}(\vec{k}, \vec{x}, t)\right), \quad (5)$$

where  $\epsilon_F(\vec{x}, t)$  is a position-dependent Fermi energy (imref) measured from some constant reference (e.g., vacuum), and  $\epsilon_{Pj}$  marks the minimum energy of the  $j$ th pocket. The corresponding equilibrium distribution is

$$f_0^{(j)}(\vec{k}) = \theta\left(\epsilon_F - \epsilon_{Pj} - \frac{\hbar^2}{2} (\vec{k} - \vec{k}_{0j})_\alpha [m_j^{-1}]_{\alpha\beta} (\vec{k} - \vec{k}_{0j})_\beta\right), \quad (6)$$

where  $\epsilon_F$  is the equilibrium Fermi energy. We can relate the density  $n_0^{(j)}$  to  $\epsilon_F$  by introducing the density-of-states mass  $\mu = [m_t^2 m_l]^{1/3}$  and the quantity  $k_{Fj}^2 = 2\mu\Delta\epsilon_{Fj}/\hbar^2$ , where  $\Delta\epsilon_{Fj} = \epsilon_F - \epsilon_{Pj}$  (i.e., the Fermi wave vector of pocket  $j$ ), and by integrating the distribution over  $k$ -space in the usual way. This gives

$$n_0^{(j)} = \frac{k_{Fj}^3}{3\pi^2}. \quad (7)$$

We can likewise define the deviation from equilibrium in the usual way:

$$\delta f^{(j)}(\vec{k}, \vec{x}, t) = f^{(j)}(\vec{k}, \vec{x}, t) - f_0^{(j)}(\vec{k}). \quad (8)$$

By integrating only over  $k$ -space, we obtain the perturbed and unperturbed hydrodynamic particle densities and their difference:

$$\begin{aligned} n^{(j)}(\vec{x}, t) &= \frac{2}{(2\pi)^3} \int d^3k f^{(j)}(\vec{k}, \vec{x}, t), \\ n_0^{(j)} &= \frac{2}{(2\pi)^3} \int d^3k f_0^{(j)}(\vec{k}), \\ \delta n^{(j)}(\vec{x}, t) &= n^{(j)}(\vec{x}, t) - n_0^{(j)}. \end{aligned} \quad (9)$$

Note that these also enter into the number-conserving collisional relaxation term and hence must be determined self-consistently. These equations couple to the Poisson equation in the usual way:

$$\nabla^2\phi = \frac{1}{\epsilon} \sum_j e_j \delta n^{(j)}(\vec{x}, t), \quad (10)$$

where the charge  $e_j = +1$  for holes,  $-1$  for electrons.

Let us linearize the Boltzmann equations around the unperturbed distributions:

$$\partial_t \delta f^{(j)} + v_\alpha^{(j)}(\vec{k}) \partial_\alpha \delta f^{(j)} + \frac{e}{\hbar} (\partial_\alpha \phi) \left( \frac{\partial}{\partial k_\alpha} f_0^{(j)}(\vec{k}) \right) = -\frac{1}{\tau_j} \left( \delta f^{(j)} - \frac{\delta n^{(j)}}{n_0^{(j)}} f_0^{(j)}(\vec{k}) \right), \quad (11)$$

where we neglect all spatial dependences to zero order. To solve these equations, we use the (wave) ansatz

$$\begin{aligned}\delta f^{(j)}(\vec{k}, \vec{x}, t) &= \delta f_q^{(j)}(\vec{k}) e^{i(\vec{q} \cdot \vec{x} - \omega t)}, \\ \delta n_q^{(j)}(\vec{x}, t) &= \delta n_q^{(j)} e^{i(\vec{q} \cdot \vec{x} - \omega t)}, \\ \phi_q &= -\frac{1}{\epsilon q^2} \sum_j e_j \delta n_q^{(j)}.\end{aligned}\quad (12)$$

Then the equations for the perturbed system become

$$\left(-i\omega + \frac{1}{\tau_j}\right) \delta f_q^{(j)}(\vec{k}) + i q_\alpha v_\alpha^{(j)}(\vec{k}) \delta f_q^{(j)}(\vec{k}) = -\frac{e_j}{\hbar} (iq_\alpha \phi_q) \left(\frac{\partial}{\partial k_\alpha} f_0^{(j)}(\vec{k})\right) + \frac{1}{\tau_j} \left(\frac{\delta n_q^{(j)}}{n_0^{(j)}} f_0^{(j)}(\vec{k})\right), \quad (13)$$

which are easily solved:

$$\delta f_q^{(j)}(\vec{k}) = \frac{\frac{e_j}{\hbar} (q_\beta \phi_q) \left(\frac{\partial}{\partial k_\beta} f_0^{(j)}(\vec{k})\right) + \frac{i}{\tau_j} \left(\frac{1}{n_0^{(j)}} f_0^{(j)}(\vec{k})\right) \delta n_q^{(j)}}{\omega + \frac{i}{\tau_j} - q_\alpha v_\alpha^{(j)}(\vec{k})}. \quad (14)$$

We can now substitute this expression back into the density expression

$$\delta n_q^{(j)} = \frac{2}{(2\pi)^3} \int \delta f_q^{(j)}(\vec{k}) d^3k \quad (15)$$

to get

$$\delta n_q^{(j)} = \frac{e_j}{\hbar} (q_\beta \phi_q) \frac{2}{(2\pi)^3} \int \frac{\frac{\partial}{\partial k_\beta} f_0^{(j)}(\vec{k})}{\omega + \frac{i}{\tau_j} - q_\alpha v_\alpha^{(j)}(\vec{k})} d^3k + \frac{i}{\tau_j} \frac{\delta n_q^{(j)}}{n_0^{(j)}} \frac{2}{(2\pi)^3} \int \frac{f_0^{(j)}(\vec{k})}{\omega + \frac{i}{\tau_j} - q_\alpha v_\alpha^{(j)}(\vec{k})} d^3k, \quad (16)$$

which can be written

$$\delta n_q^{(j)} = \frac{e_j}{\hbar} (q_\beta \phi_q) \mathfrak{I}_{1j}^\beta + \frac{i}{\tau_j} \frac{\delta n_q^{(j)}}{n_0^{(j)}} \mathfrak{I}_{2j}. \quad (17)$$

The first term in this expression contains the vector coefficient

$$\mathfrak{I}_{1j}^\beta = \frac{2}{(2\pi)^3} \int d^3k \frac{\frac{\partial}{\partial k_\beta} f_0^{(j)}(\vec{k})}{\omega + \frac{i}{\tau_j} - q_\alpha v_\alpha^{(j)}(\vec{k})}, \quad (18)$$

while the second term contains the scalar coefficient

$$\mathfrak{I}_{2j} = \frac{2}{(2\pi)^3} \int d^3\xi \frac{f_0^{(j)}(\vec{\xi})}{\omega + \frac{i}{\tau_j} - q_\alpha v_\alpha^{(j)}(\vec{\xi})}. \quad (19)$$

Since each  $k$ -space pocket in the semimetal is ellipsoidal, the hydrodynamic velocities can be defined in terms of the effective mass tensors:

$$v_{\alpha}^{(j)}(\vec{k}) = \hbar \left[ m_j^{-1} \right]_{\alpha\gamma} (\vec{k} - \vec{k}_{0j})_{\gamma} \equiv \hbar \left[ m_j^{-1} \right]_{\alpha\gamma} \xi_{\gamma}, \quad (20)$$

where  $\vec{\xi}_{\gamma}$  is the deviation in  $k$  from the  $j$ th band minimum (or maximum). Then the scalar term becomes

$$\mathfrak{S}_{2j}^{\beta} = \frac{2}{(2\pi)^3} \int d^3\xi \frac{f_0^{(j)}(\vec{\xi})}{\omega + \frac{i}{\tau_j} - q_{\alpha}\hbar \left[ m_j^{-1} \right]_{\alpha\gamma} \xi_{\gamma}}, \quad (21)$$

and the vector term becomes

$$\mathfrak{S}_{1j}^{\beta} = \frac{2}{(2\pi)^3} \int d^3\xi \frac{\frac{\partial}{\partial\xi_{\beta}} f_0^{(j)}(\vec{\xi})}{\omega + \frac{i}{\tau_j} - q_{\alpha}\hbar \left[ m_j^{-1} \right]_{\alpha\gamma} \xi_{\gamma}}. \quad (22)$$

Using the Fermi distributions

$$f_0^{(j)}(\vec{\xi}) = \theta \left( \epsilon_F - \epsilon_{Pj} - \frac{\hbar^2}{2} \xi_{\alpha} \left[ m_j^{-1} \right]_{\alpha\beta} \xi_{\beta} \right) \quad (23)$$

gives

$$\frac{\partial}{\partial\xi_{\alpha}} f_0^{(j)}(\vec{\xi}) = -\hbar^2 \left[ m_j^{-1} \right]_{\alpha\beta} \xi_{\beta} \delta \left( \epsilon_F - \epsilon_{Pj} - \frac{\hbar^2}{2} \xi_{\alpha} \left[ m_j^{-1} \right]_{\alpha\beta} \xi_{\beta} \right). \quad (24)$$

Then  $\mathfrak{S}_{1j}^{\beta}$  becomes

$$\mathfrak{S}_{1j}^{\beta} = -\hbar \frac{2}{(2\pi)^3} \int d^3\xi \frac{\hbar \left[ m_j^{-1} \right]_{\beta\gamma} \epsilon_{\gamma}}{\omega + \frac{i}{\tau_j} - q_{\alpha}\hbar \left[ m_j^{-1} \right]_{\alpha\gamma} \xi_{\gamma}} \delta(\epsilon_F - \epsilon_{\xi j}) \quad (25)$$

where

$$\epsilon_{\xi j} = \epsilon_{Pj} + \frac{\hbar^2}{2} \xi_{\alpha} \left[ m_j^{-1} \right]_{\alpha\beta} \xi_{\beta}. \quad (26)$$

We can now solve the density equation

$$\left[ 1 - \frac{i}{\tau_j} \frac{\mathfrak{S}_{2j}}{n_0^{(j)}} \right] \delta n_q^{(j)} = \frac{e_j}{\hbar} (q_{\beta} \phi_q) \mathfrak{S}_{1j}^{\beta}, \quad (27)$$

and insert the results into Poisson's equation to get

$$\phi_q = -\frac{e^2}{\epsilon q^2} \phi_q \sum_j \left[ 1 - \frac{i}{\tau_j} \frac{\mathfrak{S}_{2j}}{n_0^{(j)}} \right]^{-1} \frac{1}{\hbar} q_{\beta} \mathfrak{S}_{1j}^{\beta}. \quad (28)$$

Note that  $e_j^2 = e^2$  for solid-state systems. Equation (28) can only be true if

$$1 = -\frac{e^2}{\epsilon q^2} \sum_j \left[ 1 - \frac{i}{\tau_j} \frac{\mathfrak{S}_{2j}}{n_0^{(j)}} \right]^{-1} \frac{1}{\hbar} q_{\beta} \mathfrak{S}_{1j}^{\beta}, \quad (29)$$

where

$$q_\beta \Im_{1j}^\beta = -\hbar \frac{2}{(2\pi)^3} \int d^3\xi \frac{\hbar q_\beta [m_j^{-1}]_{\beta\gamma} \xi_\gamma}{\omega + \frac{i}{\tau_j} - \hbar q_\beta [m_j^{-1}]_{\beta\gamma} \xi_\gamma} \delta(\epsilon_F - \epsilon_{\xi j}) . \quad (30)$$

The roots of this equation define various dispersion relations for plasma waves  $\omega^{(s)}(\vec{q})$ .

Because of the  $\delta$ -function, it is possible to evaluate expression (30) analytically. Write

$$[m_j^{-1}]_{\alpha\beta} = \bar{S}_{\alpha\lambda} D_{\lambda\nu} S_{\nu\beta} , \quad (31)$$

where the matrix  $S$  is a rotation chosen to diagonalize  $m_j^{-1}$ . Then

$$q_\beta \Im_{1j}^\beta = -\hbar \frac{2}{(2\pi)^3} \int d^3\xi \frac{\hbar q_\beta S_{\beta\lambda} D_{\lambda\nu} S_{\nu\gamma} \xi_\gamma}{\omega + \frac{i}{\tau_j} - \hbar q_\beta S_{\beta\lambda} D_{\lambda\nu} S_{\nu\gamma} \xi_\gamma} \delta\left(\Delta\epsilon_{Fj} - \frac{\hbar^2}{2} \xi_\beta S_{\beta\lambda} D_{\lambda\nu} S_{\nu\gamma} \xi_\gamma\right) , \quad (32)$$

where  $\Delta\epsilon_{Fj} = \epsilon_F - \epsilon_{Pj}$ . Let  $x_\nu = S_{\nu\gamma} \xi_\gamma$ ,  $Q_\nu = S_{\nu\gamma} q_\gamma$ . Then the Jacobian for this transformation is 1, and so

$$q_\beta \Im_{1j}^\beta = -\hbar \frac{2}{(2\pi)^3} \int d^3x \frac{\hbar Q_\lambda D_{\lambda\nu} x_\nu}{\omega + \frac{i}{\tau_j} - \hbar Q_\lambda D_{\lambda\nu} x_\nu} \delta\left(\Delta\epsilon_{Fj} - \frac{\hbar^2}{2} x_\lambda D_{\lambda\nu} x_\nu\right) . \quad (33)$$

Now, since  $D$  is diagonal, we can easily define  $D = D^{1/2} D^{1/2}$  as a scaling transformation. If  $y_\nu = [D^{1/2}]_{\nu\gamma} x_\gamma$ ,  $\Lambda_\nu = \hbar [D^{1/2}]_{\nu\gamma} Q_\gamma$ , then

$$q_\beta \Im_{1j}^\beta = -\hbar [m_t^2 m_l]^{1/2} \frac{2}{(2\pi)^3} \int d^3y \frac{\Lambda_\nu y_\nu}{\omega + \frac{i}{\tau_j} - \Lambda_\nu y_\nu} \delta\left(\Delta\epsilon_{Fj} - \frac{\hbar^2}{2} y^2\right) , \quad (34)$$

where the factor in front is the Jacobian of the scaling transformation. In spherical coordinates, this expression becomes

$$q_\beta \Im_{1j}^\beta = -\frac{\hbar}{2\pi^2} [m_t^2 m_l]^{1/2} \int_0^\infty y^2 dy \delta\left(\Delta\epsilon_{Fj} - \frac{\hbar^2}{2} y^2\right) \int_{-1}^1 d(\cos\theta) \frac{\Lambda y \cos\theta}{\omega + \frac{i}{\tau_j} - \Lambda y \cos\theta} , \quad (35)$$

where

$$\Lambda = \left[ \hbar^2 \left( \frac{q_\perp^2}{m_t} + \frac{q_z^2}{m_l} \right) \right]^{1/2} = \left[ \hbar^2 q_\alpha (m_j^{-1})_{\alpha\beta} q_\beta \right]^{1/2} . \quad (36)$$

Here,  $q_\perp$  and  $q_z$  are components of  $q$  perpendicular and parallel to the  $c$ -axis of the particle material in the principal-axis system of cylindrical coordinates. I have used the fact that as a scalar  $|\Lambda|$  must be rotationally invariant. Introducing the density-of-states mass  $\mu = [m_t^2 m_l]^{1/3}$  and the Fermi wave vector  $k_{Fj}^2 = 2\mu\Delta\epsilon_{Fj}/\hbar^2$  for pocket  $j$  as we did above, we obtain

$$q_\beta \Im_{1j}^\beta = -\frac{\mu k_{Fj}}{2\pi^2 \hbar} \int_{-1}^1 d\xi \frac{\xi}{\Gamma - \xi} , \quad (37)$$

where

$$\Gamma = \frac{\omega + \frac{1}{\tau_j}}{\left[ 2\Delta\epsilon_{Fj} \left( q_\alpha \left( m_j^{-1} \right)_{\alpha\beta} q_\beta \right) \right]^{1/2}} \quad (38)$$

contains the tensor nature of the effective mass both explicitly and implicitly through the Fermi energy. The integral is trivial:

$$q_\beta \mathfrak{S}_{1j}^\beta = \frac{\mu k_{Fj}}{2\pi^2 \hbar} \left\{ 2 - \Gamma \ln \left( \frac{\Gamma + 1}{\Gamma - 1} \right) \right\} \equiv \frac{\mu k_{Fj}}{\pi^2 \hbar} f_1(\Gamma). \quad (39)$$

The quantity  $\mathfrak{S}_{2j}$  can also be evaluated explicitly. Analysis similar to that given above leads to the double integral

$$\mathfrak{S}_{2j} = \frac{1}{2\pi^2} \left[ m_t^2 m_l \right]^{1/2} \int_0^\infty y^2 dy \theta \left( \Delta\epsilon_{Fj} - \frac{\hbar^2}{2} y^2 \right) \int_{-1}^1 d(\cos \theta) \frac{1}{\omega + \frac{i}{\tau_j} - \Lambda y \cos \theta}. \quad (40)$$

Introducing the notation  $y_F = \sqrt{\frac{2\Delta\epsilon_F}{\hbar^2}}$  and  $\epsilon = \cos \theta$  as before, and using the properties of the Fermi function, we can rewrite the above as

$$\mathfrak{S}_{2j} = \frac{1}{2\pi^2} \left[ m_t^2 m_l \right]^{1/2} \int_0^{y_F} y^2 dy \int_{-1}^1 d\xi \frac{1}{\omega + \frac{i}{\tau_j} - \Lambda y \xi}. \quad (41)$$

Some algebra gives the following expression for this integral:

$$\mathfrak{S}_{2j} = \frac{3n_0^{(j)}}{2 \left( \omega + \frac{i}{\tau_j} \right)} \left\{ \Gamma^2 + (1 - \Gamma^2) \frac{\Gamma}{2} \ln \left( \frac{\Gamma + 1}{\Gamma - 1} \right) \right\} \equiv \frac{n_0^{(j)}}{\omega + \frac{i}{\tau_j}} f_2(\Gamma), \quad (42)$$

where  $\Gamma$  is the quantity introduced above.

Let us solve the plasma dispersion relation to lowest order in  $q$ , i.e., the long-wavelength limit. To do so, we take the small- $q$  limit of our explicit expressions in equations (30) and (42), which corresponds to  $\Gamma \rightarrow \infty$ . Some algebra shows that the function  $f_2(\Gamma)$  defined in equation (42) goes to 1 in this limit, so to lowest order

$$\mathfrak{S}_{2j} = \frac{1}{\omega + \frac{i}{\tau_j}} \int d^3\xi f_0^{(j)}(\xi) = \frac{n_0^{(j)}}{\omega + \frac{i}{\tau_j}}. \quad (43)$$

The same limit for  $q_\beta \mathfrak{S}_{1j}^\beta$  gives

$$q_\beta \mathfrak{S}_{1j}^\beta \approx \frac{\mu k_{Fj}}{\pi^2 \hbar} \left\{ -\frac{1}{3\Gamma^2} \right\} = -\frac{2\mu k_{Fj}}{3\pi^2 \hbar} \left\{ \frac{\Delta\epsilon_{Fj} \left( \frac{q_t^2}{m_t} + \frac{q_z^2}{m_l} \right)}{\left( \omega + i/\tau_j \right)^2} \right\}. \quad (44)$$

But

$$\begin{aligned}
-\frac{2\mu\Delta\epsilon_{Fj}k_{Fj}}{3\pi^2\hbar}\left\{\frac{\frac{q_1^2}{m_l}+\frac{q_z^2}{m_l}}{(\omega+i/\tau_j)^2}\right\} &= -\hbar^2\frac{2\mu\Delta\epsilon_{Fj}}{\hbar^2}\frac{k_{FJ}}{3\pi^2}\left\{\frac{\frac{q_1^2}{m_l}+\frac{(q_z^2)}{m_l}}{(\omega+i/\tau_j)^2}\right\} \\
&= -\hbar\frac{k_{Fj}^3}{3\pi^2}\left\{\frac{q_\alpha[m_j^{-1}]_{\alpha\beta}q_\beta}{(\omega+i/\tau_j)^2}\right\} \\
&= -\hbar n_0^{(j)}\left\{\frac{q_\alpha[m_j^{-1}]_{\alpha\beta}q_\beta}{(\omega+i/\tau_j)^2}\right\}. \quad (45)
\end{aligned}$$

so that equation (29) becomes

$$1 = \frac{e^2}{\epsilon q^2} \sum_j \left[ 1 - \frac{i}{\tau_j} \frac{1}{\omega + \frac{i}{\tau_j}} \right]^{-1} \frac{n_0^{(j)}}{\left(\omega + \frac{i}{\tau_j}\right)^2} q_\alpha [m_j^{-1}]_{\alpha\beta} q_\beta. \quad (46)$$

Assuming that the relaxation times are the same for all the pockets, we obtain

$$1 - \frac{e^2}{\epsilon q^2} \frac{1}{\omega \left(\omega + \frac{i}{\tau}\right)} q_\alpha \left\{ \sum_j n_0^{(j)} [m_j^{-1}] \right\}_{\alpha\beta} q_\beta \quad (47)$$

or, introducing the unit vector  $\hat{q} = \vec{q}/|\vec{q}|$ ,

$$1 - \frac{e^2}{\epsilon} \frac{1}{\omega \left(\omega + \frac{i}{\tau}\right)} \sum_j \left\{ n_0^{(j)} \hat{q}_\alpha [m_j^{-1}]_{\alpha\beta} \hat{q}_\beta \right\} = 0. \quad (48)$$

This expression, which is clearly in the form of a requirement that a "Drude"-type conductivity for the system should vanish, defines the "plasma frequency" of the multicomponent system as the sum in the numerator. In general this sum will depend on the direction of  $\hat{q}$ .

To derive an analogue of the linearized Thomas-Fermi equation and a corresponding screening length, we need to take these expansions to higher order in  $q$ . Saving next-order terms in  $f_1(\Gamma)$  and  $f_2(\Gamma)$  gives

$$f_1(\Gamma) \approx -\frac{1}{3\Gamma^2} - \frac{1}{5\Gamma^4}, \quad f_2(\Gamma) \approx 1 + \frac{1}{5\Gamma^2}. \quad (49)$$

Let us rewrite equation (29) as

$$1 = -\frac{e^2}{\epsilon q^2} \sum_j \left[ 1 - \frac{i}{\tau_j} \frac{f_2(\Gamma)}{\omega + \frac{i}{\tau_j}} \right] \frac{\mu k_{Fj}}{\pi^2 \hbar} f_1(\Gamma) \quad (50)$$

and note that

$$\frac{\mu k_{Fj}}{\pi^2 \hbar} = \frac{3}{2} \frac{n_0^{(j)}}{\Delta\epsilon_{Fj}}. \quad (51)$$

Then equation (50) becomes

$$1 = -\frac{1}{q^2} \sum_j \lambda_j^2 \left[ 1 - \frac{i}{\tau_j} \frac{f_2(\Gamma)}{\omega + \frac{i}{\tau_j}} \right]^{-1} f_1(\Gamma), \quad (52)$$

where  $\lambda_j^2$  is the Thomas-Fermi screening length for carriers in the  $j$ th pocket:

$$\lambda_j^2 = \frac{3}{2\epsilon} \frac{n_0^{(j)} e^2}{\Delta\epsilon_{Fj}}. \quad (53)$$

With these results, we can easily derive the expression

$$1 = \sum_j \frac{n_0^{(j)} e^2}{\epsilon q^2} \frac{q_\alpha [m_j^{-1}]_{\alpha\beta} q_\beta}{\omega (\omega + \frac{i}{\tau_j})} \left[ 1 + \frac{6}{5} \frac{\Delta\epsilon_{Fj}}{\left(\omega + \frac{i}{\tau_j}\right)^2} \left( 1 + \frac{2}{3} \frac{i}{\omega\tau_j} \right) q_\alpha [m_j^{-1}]_{\alpha\beta} q_\beta \right]. \quad (54)$$

The peculiar fraction (6/5) that occurs in this expression derives from our linearization around a spatially independent zero-order distribution. A more careful linearization is needed to recover the true hydrodynamic value of this coefficient and, indeed, to recover any of the expressions encountered in classical fluid mechanics. This will be the subject of a subsequent report.

---

### 3. Calculations of Sums Over $k$ -Space Minima for High-Symmetry Band Structures

---

#### 3.1 Simple Cubic Band Structure

A simple cubic band structure is appropriate for elemental silicon (see fig. 1). In order to calculate the effective masses for this method, we assume that the densities in the carrier pockets are the same, and that the principal-axis projections are  $\hat{x}\hat{x}$ ,  $\hat{y}\hat{y}$ , and  $\hat{z}\hat{z}$ . Since there are six pockets, each holds 1/6 of the electrons.

Let us write the effective masses as follows:

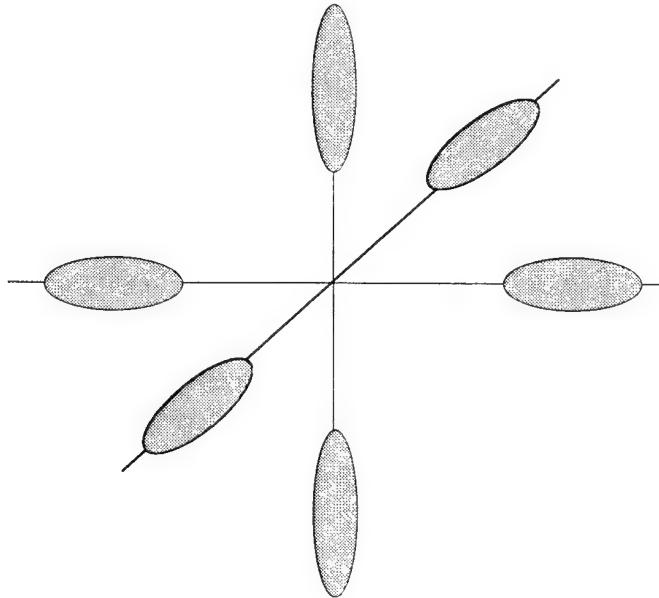
$$\begin{aligned} [m^{(1)}]^{-1} &= [m^{(-1)}]^{-1} = \frac{1}{m_l} \hat{x}\hat{x} + \frac{1}{m_t} (\hat{y}\hat{y} + \hat{z}\hat{z}) , \\ [m^{(2)}]^{-1} &= [m^{(-2)}]^{-1} = \frac{1}{m_l} \hat{y}\hat{y} + \frac{1}{m_t} (\hat{x}\hat{x} + \hat{z}\hat{z}) , \quad \text{and} \\ [m^{(3)}]^{-1} &= [m^{(-3)}]^{-1} = \frac{1}{m_l} \hat{z}\hat{z} + \frac{1}{m_t} (\hat{y}\hat{y} + \hat{x}\hat{x}) . \end{aligned} \quad (55)$$

Then the sum is simple:

$$\sum_j n_0^{(j)} [m_j^{-1}] = \frac{1}{6} n_0 \left( \frac{1}{m_l} + \frac{2}{m_t} \right) 2 [\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z}] = \frac{1}{3} n_0 \left( \frac{1}{m_l} + \frac{2}{m_t} \right) \overleftrightarrow{1} , \quad (56)$$

where  $\overleftrightarrow{1}$  is the identity matrix. This shows that the mass required is just the usual isotropic optical mass.

Figure 1. Conduction band minima (pockets) of silicon in  $k$ -space.



### 3.2 (111) Cubic Pockets (Tetrahedral Band Structure)

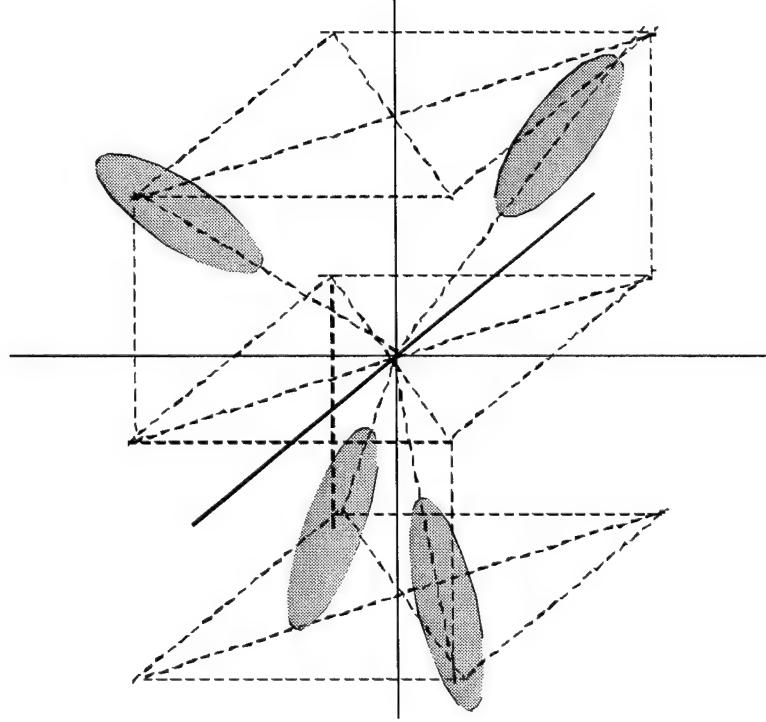
A tetrahedral band structure is appropriate for elemental germanium (see fig. 2). Here we have four pockets, at the vertices of a tetrahedron. The effective-mass tensors are

$$\begin{aligned} [m^{(1)}]^{-1} &= [m^{(-1)}]^{-1} = \frac{1}{m_l} \hat{e}_1 \hat{e}_1 + \frac{1}{m_t} (\hat{s}_1 \hat{s}_1 + \hat{t}_1 \hat{t}_1) , \\ [m^{(2)}]^{-1} &= [m^{(-2)}]^{-1} = \frac{1}{m_l} \hat{e}_2 \hat{e}_2 + \frac{1}{m_t} (\hat{s}_2 \hat{s}_2 + \hat{t}_2 \hat{t}_2) , \\ [m^{(3)}]^{-1} &= [m^{(-3)}]^{-1} = \frac{1}{m_l} \hat{e}_3 \hat{e}_3 + \frac{1}{m_t} (\hat{s}_3 \hat{s}_3 + \hat{t}_3 \hat{t}_3) , \quad \text{and} \\ [m^{(4)}]^{-1} &= [m^{(-4)}]^{-1} = \frac{1}{m_l} \hat{e}_4 \hat{e}_4 + \frac{1}{m_t} (\hat{s}_4 \hat{s}_4 + \hat{t}_4 \hat{t}_4) , \end{aligned} \quad (57)$$

where the vectors  $\hat{e}_i, \hat{s}_i, \hat{t}_i \equiv \hat{e}_i \otimes \hat{s}_i$  mark the principal axes of the pocket ellipsoids:

$$\begin{aligned} \hat{e}_1 &= \frac{1}{\sqrt{3}} (\hat{x} + \hat{y} + \hat{z}) , \quad \hat{s}_1 = \frac{1}{\sqrt{2}} (-\hat{x} + \hat{y}) , \quad \hat{t}_1 = \frac{1}{\sqrt{6}} (-\hat{x} - \hat{y} + 2\hat{z}) ; \\ \hat{e}_2 &= \frac{1}{\sqrt{3}} (-\hat{x} + \hat{y} - \hat{z}) , \quad \hat{s}_2 = \frac{1}{\sqrt{2}} (-\hat{x} - \hat{y}) , \quad \hat{t}_2 = \frac{1}{\sqrt{6}} (-\hat{x} + \hat{y} + 2\hat{z}) ; \\ \hat{e}_3 &= \frac{1}{\sqrt{3}} (-\hat{x} - \hat{y} + \hat{z}) , \quad \hat{s}_3 = \frac{1}{\sqrt{2}} (\hat{x} - \hat{y}) , \quad \hat{t}_3 = \frac{1}{\sqrt{6}} (\hat{x} + \hat{y} + 2\hat{z}) ; \quad \text{and} \\ \hat{e}_4 &= \frac{1}{\sqrt{3}} (\hat{x} - \hat{y} - \hat{z}) , \quad \hat{s}_4 = \frac{1}{\sqrt{2}} (\hat{x} + \hat{y}) , \quad \hat{t}_4 = \frac{1}{\sqrt{6}} (\hat{x} - \hat{y} + 2\hat{z}) . \end{aligned} \quad (58)$$

Figure 2. Conduction band minima (pockets) of germanium in  $k$ -space.



Then the dyadic products can be written in matrix form as follows:

$$\begin{aligned}
\hat{e}_1 \hat{e}_1 &= \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad \hat{s}_1 \hat{s}_1 = \frac{1}{2} \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{t}_1 \hat{t}_1 = \frac{1}{6} \begin{pmatrix} 1 & 1 & -2 \\ 1 & 1 & -2 \\ -2 & -2 & 4 \end{pmatrix}; \\
\hat{e}_2 \hat{e}_2 &= \frac{1}{3} \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix}, \quad \hat{s}_2 \hat{s}_2 = \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{t}_2 \hat{t}_2 = \frac{1}{6} \begin{pmatrix} 1 & -1 & -2 \\ -1 & 1 & 2 \\ -2 & 2 & 4 \end{pmatrix}; \\
\hat{e}_3 \hat{e}_3 &= \frac{1}{3} \begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}, \quad \hat{s}_3 \hat{s}_3 = \frac{1}{2} \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{t}_3 \hat{t}_3 = \frac{1}{6} \begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \\ 2 & 2 & 4 \end{pmatrix}; \\
\hat{e}_4 \hat{e}_4 &= \frac{1}{3} \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix}, \quad \hat{s}_4 \hat{s}_4 = \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{t}_4 \hat{t}_4 = \frac{1}{6} \begin{pmatrix} 1 & -1 & 2 \\ -1 & 1 & -2 \\ 2 & -2 & 4 \end{pmatrix}.
\end{aligned} \tag{59}$$

Performing the summation once more, we obtain

$$\begin{aligned}
[m^{(1)}]^{-1} &= \frac{1}{3m_l} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} + \frac{1}{m_t} \left\{ \frac{1}{2} \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{6} \begin{pmatrix} 1 & 1 & -2 \\ 1 & 1 & -2 \\ -2 & -2 & 4 \end{pmatrix} \right\} \\
&= \frac{1}{m_l} \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} + \frac{1}{m_t} \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{pmatrix},
\end{aligned}$$

$$\begin{aligned}
[m^{(2)}]^{-1} &= \frac{1}{3m_l} \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix} + \frac{1}{m_t} \left\{ \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{6} \begin{pmatrix} 1 & -1 & -2 \\ -1 & 1 & 2 \\ -2 & 2 & 4 \end{pmatrix} \right\} \\
&= \frac{1}{m_l} \begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \end{pmatrix} + \frac{1}{m_t} \begin{pmatrix} \frac{2}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{1}{3} & \frac{2}{3} \end{pmatrix},
\end{aligned}$$

$$\begin{aligned}
[m^{(3)}]^{-1} &= \frac{1}{3m_l} \begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix} + \frac{1}{m_t} \left\{ \frac{1}{2} \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{6} \begin{pmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \\ 2 & 2 & 4 \end{pmatrix} \right\} \\
&= \frac{1}{m_l} \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \end{pmatrix} + \frac{1}{m_t} \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{2}{3} \end{pmatrix},
\end{aligned} \tag{60}$$

and so

$$\begin{aligned} [m^{(4)}]^{-1} &= \frac{1}{3m_l} \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix} + \frac{1}{m_t} \left\{ \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{6} \begin{pmatrix} 1 & -1 & 2 \\ -1 & 1 & -2 \\ 2 & -2 & 4 \end{pmatrix} \right\} \\ &= \frac{1}{m_l} \begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ -\frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} + \frac{1}{m_t} \begin{pmatrix} \frac{2}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{pmatrix}. \end{aligned} \quad (61)$$

Each pocket holds 1/4 of the electrons. Then the total mass sum equals

$$\sum_j n_0^{(j)} [m_j^{-1}] = \frac{1}{4} n_0 \left\{ \frac{1}{m_l} \right\} \begin{pmatrix} \frac{4}{3} & 0 & 0 \\ 0 & \frac{4}{3} & 0 \\ 0 & 0 & \frac{4}{3} \end{pmatrix} + \frac{1}{m_t} \begin{pmatrix} \frac{8}{3} & 0 & 0 \\ 0 & \frac{8}{3} & 0 \\ 0 & 0 & \frac{8}{3} \end{pmatrix} = \frac{1}{3} n_0 \left( \frac{1}{m_l} + \frac{2}{m_t} \right) \overset{\leftrightarrow}{1}, \quad (62)$$

which is again the isotropic optical mass.

---

## 4. Calculations of Sums Over $k$ -space Minima for the Band Structures of Group-V Elements

---

The band structures of the group-V elements are described in detail by Lin and Falicov [4] and Shapira and Williamson [5]. For the conduction band, the pattern of ellipsoidal pockets shown in figure 3 is obtained; the angle with  $z$ -axis  $\theta_C$  is material-dependent. I assume here that the valence band has a similar structure, although the actual Fermi surface of As is a single multiconnected surface rather than a collection of pockets.

Let

$$\sigma = \cos \theta_C , \quad \tau = \sin \theta_C . \quad (63)$$

Then the hexagonal symmetry in the basal plane motivates us to introduce the quantities

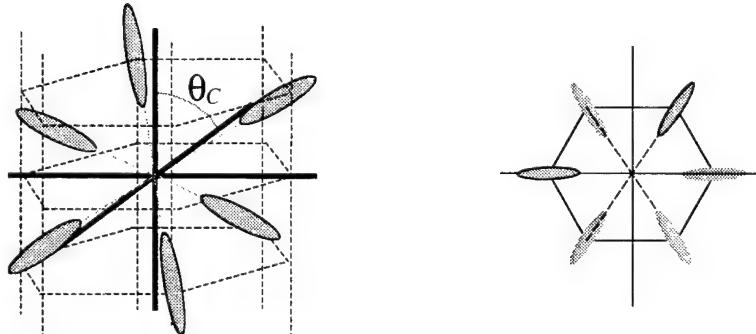
$$\alpha = 1/2 , \quad \beta = \sqrt{3}/2 . \quad (64)$$

This allows us to write the longitudinal-mass principal axis vectors as follows:

$$\begin{aligned} \hat{e}_1 &= \tau \hat{x} + \sigma \hat{z} , \\ \hat{e}_2 &= \alpha \tau \hat{x} + \beta \tau \hat{y} - \sigma \hat{z} , \\ \hat{e}_3 &= -\alpha \tau \hat{x} + \beta \tau \hat{y} + \sigma \hat{z} , \\ \hat{e}_4 &= -\tau \hat{x} - \sigma \hat{z} , \\ \hat{e}_5 &= -\alpha \tau \hat{x} - \beta \tau \hat{y} + \sigma \hat{z} , \quad \text{and} \\ \hat{e}_6 &= \alpha \tau \hat{x} - \beta \tau \hat{y} - \sigma \hat{z} . \end{aligned} \quad (65)$$

**Figure 3.**  
Conduction-band and valence-band minima (pockets) of As and Sb in  $k$ -space. Upper pockets are filled with electrons, lower ones with holes.

(a) Three-dimensional view, and (b) view down  $c$ -axis ( $z$ -axis in (a)).



Then the other principal axes are

$$\begin{aligned}\hat{s}_1 &= \hat{y}, & \hat{t}_1 &= -\sigma\hat{x} + \tau\hat{z}; \\ \hat{s}_2 &= -\beta\hat{x} + \alpha\hat{y}, & \hat{t}_2 &= \alpha\sigma\hat{x} + \beta\sigma\hat{y} + \tau\hat{z}; \\ \hat{s}_3 &= -\beta\hat{x} - \alpha\hat{y}, & \hat{t}_3 &= -\alpha\sigma\hat{x} + \beta\sigma\hat{y} - \tau\hat{z}; \\ \hat{s}_4 &= -\hat{y}, & \hat{t}_4 &= -\sigma\hat{x} + \tau\hat{z}; \\ \hat{s}_5 &= \beta\hat{x} - \alpha\hat{y}, & \hat{t}_5 &= \alpha\sigma\hat{x} + \beta\sigma\hat{y} + \tau\hat{z}; \quad \text{and} \\ \hat{s}_6 &= \beta\hat{x} + \alpha\hat{y}, & \hat{t}_6 &= \alpha\sigma\hat{x} - \beta\sigma\hat{y} + \tau\hat{z}.\end{aligned}\tag{66}$$

As before, we find the projection operators

$$\begin{aligned}\hat{e}_1\hat{e}_1 &= \begin{pmatrix} \tau^2 & 0 & \sigma\tau \\ 0 & 0 & 0 \\ \sigma\tau & 0 & \sigma^2 \end{pmatrix}, & \hat{s}_1\hat{s}_1 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \hat{t}_1\hat{t}_1 &= \begin{pmatrix} \sigma^2 & 0 & -\sigma\tau \\ 0 & 0 & 0 \\ -\sigma\tau & 0 & \tau^2 \end{pmatrix}; \\ \hat{e}_2\hat{e}_2 &= \begin{pmatrix} \alpha^2\tau^2 & \alpha\beta\tau^2 & -\alpha\tau\sigma \\ \alpha\beta\tau^2 & \beta^2\tau^2 & -\beta\tau\sigma \\ -\alpha\tau\sigma & -\beta\tau\sigma & \sigma^2 \end{pmatrix}, & \hat{s}_2\hat{s}_2 &= \begin{pmatrix} \beta^2 & -\alpha\beta & 0 \\ -\alpha\beta & \alpha^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \hat{t}_2\hat{t}_2 &= \begin{pmatrix} \alpha^2\sigma^2 & \alpha\beta\sigma^2 & \alpha\tau\sigma \\ \alpha\beta\sigma^2 & \beta^2\sigma^2 & \beta\tau\sigma \\ \alpha\tau\sigma & \beta\tau\sigma & \tau^2 \end{pmatrix}; \\ \hat{e}_3\hat{e}_3 &= \begin{pmatrix} \alpha^2\tau^2 & -\alpha\beta\tau^2 & -\alpha\tau\sigma \\ -\alpha\beta\tau^2 & \beta^2\tau^2 & \beta\tau\sigma \\ -\alpha\tau\sigma & \beta\tau\sigma & \sigma^2 \end{pmatrix}, & \hat{s}_3\hat{s}_3 &= \begin{pmatrix} \beta^2 & \alpha\beta & 0 \\ \alpha\beta & \alpha^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \hat{t}_3\hat{t}_3 &= \begin{pmatrix} \alpha^2\sigma^2 & -\alpha\beta\sigma^2 & \alpha\tau\sigma \\ -\alpha\beta\sigma^2 & \beta^2\sigma^2 & -\beta\tau\sigma \\ \alpha\tau\sigma & -\beta\tau\sigma & \tau^2 \end{pmatrix}; \\ \hat{e}_4\hat{e}_4 &= \begin{pmatrix} \tau^2 & 0 & \sigma\tau \\ 0 & 0 & 0 \\ \sigma\tau & 0 & \sigma^2 \end{pmatrix}, & \hat{s}_4\hat{s}_4 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \hat{t}_4\hat{t}_4 &= \begin{pmatrix} \sigma^2 & 0 & -\sigma\tau \\ 0 & 0 & 0 \\ -\sigma\tau & 0 & \tau^2 \end{pmatrix}; \\ \hat{e}_5\hat{e}_5 &= \begin{pmatrix} \alpha^2\tau^2 & \alpha\beta\tau^2 & -\alpha\tau\sigma \\ \alpha\beta\tau^2 & \beta^2\tau^2 & -\beta\tau\sigma \\ -\alpha\tau\sigma & -\beta\tau\sigma & \sigma^2 \end{pmatrix}, & \hat{s}_5\hat{s}_5 &= \begin{pmatrix} \beta^2 & -\alpha\beta & 0 \\ -\alpha\beta & \alpha^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \hat{t}_5\hat{t}_5 &= \begin{pmatrix} \alpha^2\sigma^2 & \alpha\beta\sigma^2 & \alpha\tau\sigma \\ \alpha\beta\sigma^2 & \beta^2\sigma^2 & \beta\tau\sigma \\ \alpha\tau\sigma & \beta\tau\sigma & \tau^2 \end{pmatrix}; \\ \hat{e}_6\hat{e}_6 &= \begin{pmatrix} \alpha^2\tau^2 & -\alpha\beta\tau^2 & -\alpha\tau\sigma \\ -\alpha\beta\tau^2 & \beta^2\tau^2 & \beta\tau\sigma \\ -\alpha\tau\sigma & \beta\tau\sigma & \sigma^2 \end{pmatrix}, & \hat{s}_6\hat{s}_6 &= \begin{pmatrix} \beta^2 & \alpha\beta & 0 \\ \alpha\beta & \alpha^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \hat{t}_6\hat{t}_6 &= \begin{pmatrix} \alpha^2\sigma^2 & -\alpha\beta\sigma^2 & \alpha\tau\sigma \\ -\alpha\beta\sigma^2 & \beta^2\sigma^2 & -\beta\tau\sigma \\ \alpha\tau\sigma & -\beta\tau\sigma & \tau^2 \end{pmatrix}.\end{aligned}\tag{67}$$

The dyadic sums are then

$$\begin{aligned}\sum_{i=1}^6 \hat{e}_i\hat{e}_i &= \begin{pmatrix} 4\alpha^2\tau^2+2\tau^2 & 0 & 2(1-2\alpha)\tau\sigma \\ 0 & 4\beta^2\tau^2 & 0 \\ 2(1-2\alpha)\tau\sigma & 0 & 6\sigma^2 \end{pmatrix}, \\ \sum_{i=1}^6 \hat{t}_i\hat{t}_i &= \begin{pmatrix} 4\alpha^2\sigma^2+2\sigma^2 & 0 & -2(1-2\alpha)\tau\sigma \\ 0 & 4\beta^2\sigma^2 & 0 \\ -2(1-2\alpha)\tau\sigma & 0 & 6\tau^2 \end{pmatrix}, \quad \text{and} \\ \sum_{i=1}^6 \hat{s}_i\hat{s}_i &= \begin{pmatrix} 4\beta^2 & 0 & 0 \\ 0 & 4\alpha^2+2 & 0 \\ 0 & 0 & 0 \end{pmatrix}.\end{aligned}\tag{68}$$

Hence,

$$\sum_{i=1}^6 \hat{s}_i\hat{s}_i + \hat{t}_i\hat{t}_i = \begin{pmatrix} 4\beta^2+4\alpha^2\sigma^2+2\sigma^2 & 0 & -2(1-2\alpha)\tau\sigma \\ 0 & 4\alpha^2+4\beta^2\sigma^2+2 & 0 \\ -2(1-2\alpha)\tau\sigma & 0 & 6\tau^2 \end{pmatrix}.\tag{69}$$

Note that because  $\alpha = 1/2$ , this tensor is diagonal! Since  $\beta^2 = 3/4$ , the above

becomes

$$\sum_{i=1}^6 \hat{s}_i \hat{s}_i + \hat{t}_i \hat{t}_i = \begin{pmatrix} 3(1+\sigma^2) & 0 & 0 \\ 0 & 3(1+\sigma^2) & 0 \\ 0 & 0 & 6\tau^2 \end{pmatrix}. \quad (70)$$

Likewise, we have

$$\sum_{i=1}^6 \hat{e}_i \hat{e}_i = \begin{pmatrix} 3\tau^2 & 0 & 0 \\ 0 & 3\tau^2 & 0 \\ 0 & 0 & 6\sigma^2 \end{pmatrix} \quad (71)$$

so that the averaged optical effective-mass tensor is

$$\begin{aligned} \sum_j n_0^{(j)} [m_j^{-1}] &= \frac{1}{6} n_0 \left\{ \frac{1}{m_l} \begin{pmatrix} 3\tau^2 & 0 & 0 \\ 0 & 3\tau^2 & 0 \\ 0 & 0 & 6\sigma^2 \end{pmatrix} + \frac{1}{m_t} \begin{pmatrix} 3(1+\sigma^2) & 0 & 0 \\ 0 & 3(1+\sigma^2) & 0 \\ 0 & 0 & 6\tau^2 \end{pmatrix} \right\} \\ &= \frac{1}{2} n_0 \begin{pmatrix} \frac{1}{m_l} \tau^2 + \frac{1}{m_t} (1+\sigma^2) & 0 & 0 \\ 0 & \frac{1}{m_l} \tau^2 + \frac{1}{m_t} (1+\sigma^2) & 0 \\ 0 & 0 & \frac{1}{m_l} \sigma^2 + \frac{1}{m_t} \tau^2 \end{pmatrix}. \end{aligned} \quad (72)$$

In keeping with our expectations, the effective mass tensor is somewhat anisotropic. However, there is an angle at which it becomes isotropic; this is

$$\cos 2\theta_C = \frac{m_l}{m_t - m_l}. \quad (73)$$

It is easy to show that the reported angles for the group-V materials do not satisfy this criterion, so that anisotropy will be a real issue in any study of their plasma response.

---

## 5. Conclusions

---

In this report, certain properties of the multicomponent plasmas present in the group-V semimetals As, Sb, and Bi have been derived. Notable among these properties is anisotropy of the effective masses of both electrons and holes, which in turn leads to anisotropy in the plasma frequencies of these materials. Because the systems of interest are particles in a host matrix rather than bulk materials, it is likely that this anisotropy in the plasma response will be averaged out in some way; however, this problem must be examined in detail before such a conclusion is warranted.

---

## References

---

1. J. M. Ziman, *Principles of the Theory of Solids*, ch. 4, Cambridge University Press, Cambridge (1964).
2. Z. Liliental-Weber, A. Claverie, J. Washburn, F. Smith, and R. Calawa, "Microstructure of Annealed Low-Temperature-Grown GaAs Layers," *Appl. Phys. A* **53** (1991), 141.
3. K. Bløtekjær, "Transport Equations for Electrons in Two-Valley Semiconductors," *IEEE Trans. Electron Devices* **ED-17** (1970), 38.
4. P. J. Lin and L. M. Falicov, "Fermi Surface of Arsenic," *Phys. Rev.* **142** (1966), 441.
5. Y. Shapira and S. J. Williamson, "Quantum Oscillations in the Ultrasonic Attenuation and Magnetic Susceptibility of Arsenic," *Phys. Lett.* **14** (1965), 73.

## Distribution

Admnstr  
Defns Techl Info Ctr  
Attn DTIC-OCP  
8725 John J Kingman Rd Ste 0944  
FT Belvoir VA 22060-6218

Ofc of the Secy of Defns  
Attn ODDRE (R&AT)  
The Pentagon  
Washington DC 20301-3080

Ofc of the Secy of Defns  
Attn OUSD(A&T)/ODDR&E(R) R J Trew  
3080 Defense Pentagon  
Washington DC 20301-7100

AMCOM MRDEC  
Attn AMSMI-RD W C McCorkle  
Redstone Arsenal AL 35898-5240

CECOM  
Attn PM GPS COL S Young  
FT Monmouth NJ 07703

DARPA  
Attn DARPA/MTO E Martinez  
3701 N Fairfax Dr  
Arlington VA 22203-1714

Dir for MANPRINT  
Ofc of the Deputy Chief of Staff for Prsnnl  
Attn J Hiller  
The Pentagon Rm 2C733  
Washington DC 20301-0300

US Army ARDEC  
Attn AMSTA-AR-TD M Fisette  
Bldg 1  
Picatinny Arsenal NJ 07806-5000

US Army Info Sys Engrg Cmnd  
Attn ASQB-OTD F Jenia  
FT Huachuca AZ 85613-5300

US Army Natick RDEC Acting Techl Dir  
Attn SSCNC-T P Bandler  
Natick MA 01760-5002

US Army Simulation, Train, & Instrmntn  
Cmnd  
Attn J Stahl  
12350 Research Parkway  
Orlando FL 32826-3726

US Army Soldier & Biol Chem Cmnd Dir of  
Rsrch & Techlgry Dirctr  
Attn SMCCR-RS IG Resnick  
Aberdeen Proving Ground MD 21010-5423

US Army Tank-Automtv Cmnd Rsrch, Dev, &  
Engrg Ctr  
Attn AMSTA-TR J Chapin  
Warren MI 48397-5000

US Army Train & Doctrine Cmnd  
Battle Lab Integration & Techl Dirctr  
Attn ATCD-B J A Klevecz  
FT Monroe VA 23651-5850

US Military Academy  
Mathematical Sci Ctr of Excellence  
Attn MDN-A LTC M D Phillips  
Dept of Mathematical Sci Thayer Hall  
West Point NY 10996-1786

Nav Surface Warfare Ctr  
Attn Code B07 J Pennella  
17320 Dahlgren Rd Bldg 1470 Rm 1101  
Dahlgren VA 22448-5100

DARPA  
Attn S Welby  
3701 N Fairfax Dr  
Arlington VA 22203-1714

Univ of Maryland Lab for Physical Sci  
Attn K Ritter  
Attn W Beard  
College Park MD 20742

Hicks & Associates Inc  
Attn G Singley III  
1710 Goodrich Dr Ste 1300  
McLean VA 22102

## Distribution (cont'd)

Palisades Inst for Rsrch Svc Inc  
Attn E Carr  
1745 Jefferson Davis Hwy Ste 500  
Arlington VA 22202-3402

US Army Rsrch Lab  
Attn AMSRL-SL-BN J Soln  
Aberdeen Proving Ground MD 21005

Director  
US Army Rsrch Ofc  
Attn H Everitt  
Attn AMSRL-RO M Stroscio  
Attn D Wolard  
Attn J Harvey  
Attn J Prater  
Attn M Dutta  
Attn AMSRL-RO-D JCI Chang  
PO Box 12211  
Research Triangle Park NC 27709

US Army Rsrch Lab  
Attn AMSRL-DD J M Miller  
Attn AMSRL-CI-AI-R Mail & Records Mgmt  
Attn AMSRL-CI-AP Techl Pub (3 copies)  
Attn AMSRL-CI-LL Techl Lib (3 copies)  
Attn AMSRL-SE E Poindexter  
Attn AMSRL-SE J M McGarrity  
Attn AMSRL-SE J Pellegrino  
Attn AMSRL-SE-DP A Bromborsky  
Attn AMSRL-SE-DP H Brandt  
Attn AMSRL-SE-DP R del Rosario  
Attn AMSRL-SE-DS C Fazi  
Attn AMSRL-SE-E H Pollehn  
Attn AMSRL-SE-E J Mait  
Attn AMSRL-SE-E W Clark  
Attn AMSRL-SE-EE A Goldberg  
Attn AMSRL-SE-EE D Beekman  
Attn AMSRL-SE-EE M Patterson

US Army Rsrch Lab (cont'd)  
Attn AMSRL-SE-EE S Kennerly  
Attn AMSRL-SE-EE Z G Sztankay  
Attn AMSRL-SE-EI B Beck  
Attn AMSRL-SE-EI J Little  
Attn AMSRL-SE-EI K K Choi  
Attn AMSRL-SE-EI M Tidrow  
Attn AMSRL-SE-EI N Dhar  
Attn AMSRL-SE-EI R Leavitt  
Attn AMSRL-SE-EI T Zheleva  
Attn AMSRL-SE-EM G Simonis  
Attn AMSRL-SE-EM J Pamulapati  
Attn AMSRL-SE-EM M Tobin  
Attn AMSRL-SE-EM P Shen  
Attn AMSRL-SE-EM W Chang  
Attn AMSRL-SE-EO N Gupta  
Attn AMSRL-SE-EP D Wortman  
Attn AMSRL-SE-EP J Bradshaw  
Attn AMSRL-SE-EP J Bruno  
Attn AMSRL-SE-EP M Wraback  
Attn AMSRL-SE-EP P Folkes  
Attn AMSRL-SE-EP R Tober  
Attn AMSRL-SE-EP S Rudin  
Attn AMSRL-SE-EP T B Bahder  
Attn AMSRL-SE-EP T Oldham  
Attn AMSRL-SE-R B Wallace  
Attn AMSRL-SE-RE F Crowne (5 copies)  
Attn AMSRL-SE-RE R Chase  
Attn AMSRL-SE-RE R Kaul  
Attn AMSRL-SE-RE S Tidrow  
Attn AMSRL-SE-RL C Scozzie  
Attn AMSRL-SE-RL A Lepore  
Attn AMSRL-SE-RL M Dubey  
Attn AMSRL-SE-RL S Svensson  
Attn AMSRL-SE-SS K Jones  
Adelphi MD 20783-1197

<b>REPORT DOCUMENTATION PAGE</b>			<i>Form Approved OMB No. 0704-0188</i>
<p>Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.</p>			
1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE August 2000	3. REPORT TYPE AND DATES COVERED Interim, 1/99-9/99	
4. TITLE AND SUBTITLE Derivation of Effective-Mass Expressions for Electrons and Holes in the Anisotropic Multiband Semimetals Ar, Sb, and Bi			5. FUNDING NUMBERS DA PR: AH94 PE: 62120A
6. AUTHOR(S) Frank J. Crowne			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory Attn: AMSRL-SE-RE email: fcrown@arl.mil 2800 Powder Mill Road Adelphi, MD 20783-1197			8. PERFORMING ORGANIZATION REPORT NUMBER ARL-TR-2152
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory 2800 Powder Mill Road Adelphi, MD 20783-1197			10. SPONSORING/MONITORING AGENCY REPORT NUMBER
11. SUPPLEMENTARY NOTES ARL PR: ONE6K1 AMS code: 622705.H94			
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.			12b. DISTRIBUTION CODE
13. ABSTRACT (Maximum 200 words) In this report, certain properties of the multicomponent plasmas present in the group-V semimetals As, Sb, and Bi have been derived. Notable among these properties is anisotropy of the effective masses of both electrons and holes, which in turn leads to anisotropy in the plasma frequencies of these materials. Because the systems of interest are particulates in a host matrix rather than bulk materials, it is likely that this anisotropy in the plasma response will be averaged out in some way; however, this problem must be examined in detail before such a conclusion is warranted.			
14. SUBJECT TERMS Semimetals, effective mass, plasma frequency			15. NUMBER OF PAGES 26
			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT UL